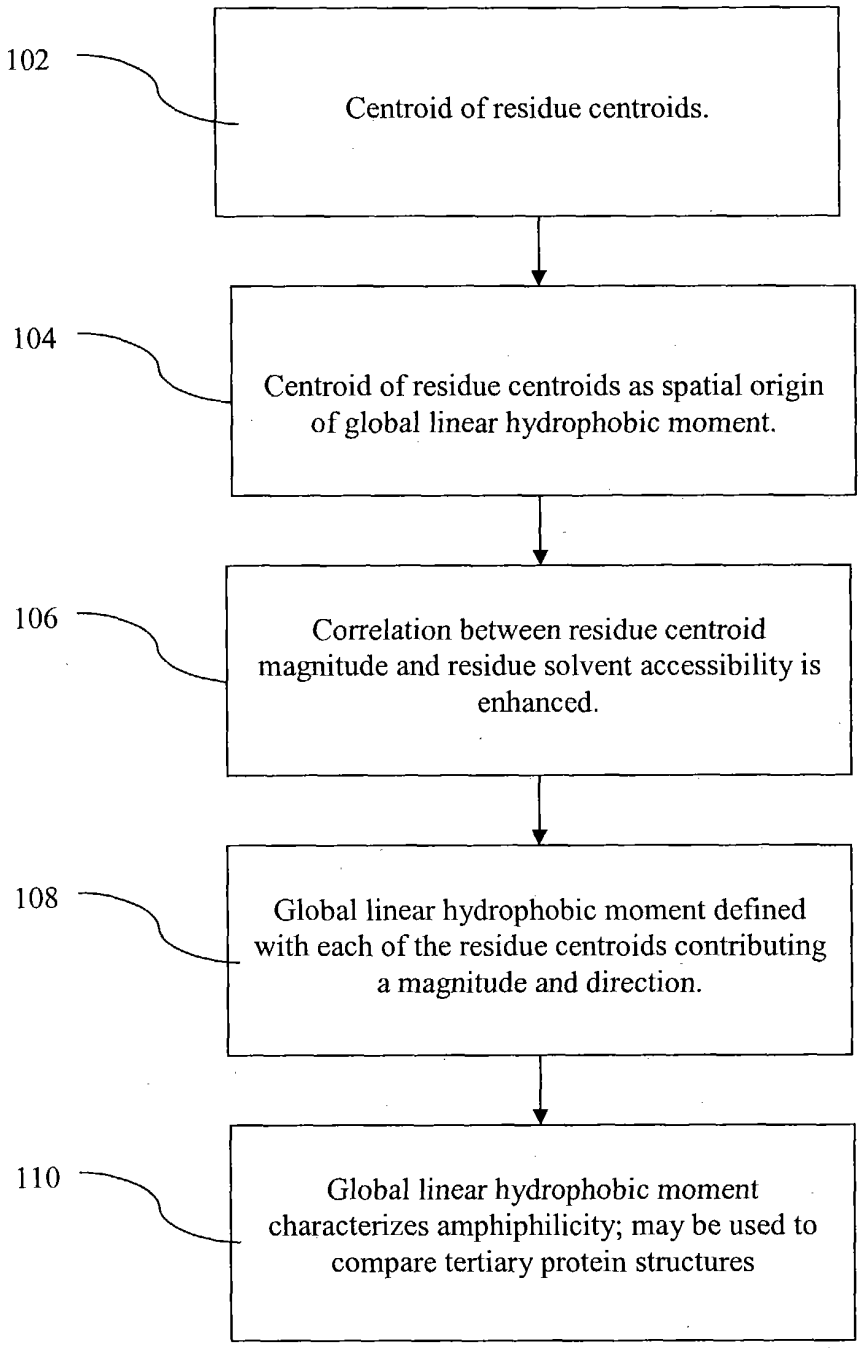
102
Centroid of residue centroids.
104
Centroid of residue centroids as spatial origin of global linear hydrophobic moment.
106
Correlation between residue centroid magnitude and residue solvent accessibility is enhanced.
108
Global linear hydrophobic moment defined with each of the residue centroids contributing a magnitude and direction.
110
Global linear hydrophobic moment characterizes amphiphilicity; may be used to compare tertiary protein structures

FIG. 1

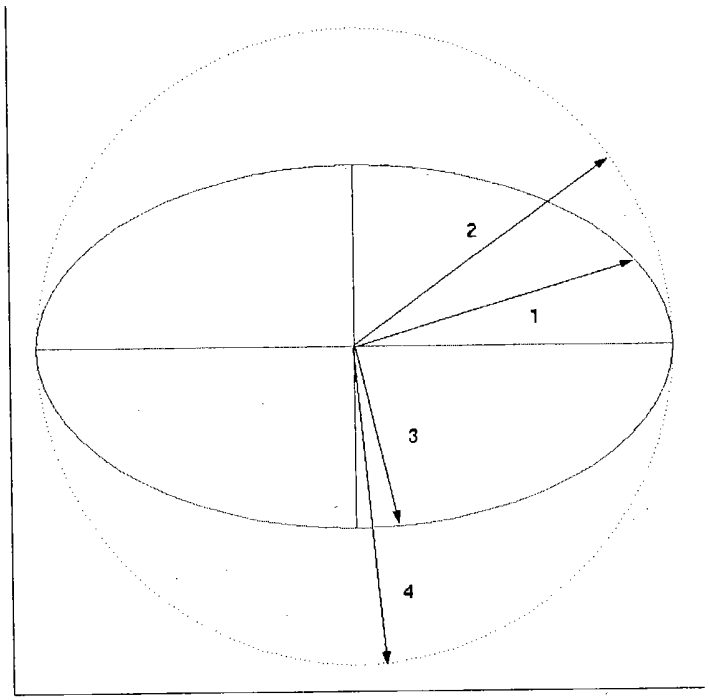

FIG. 2

Correlation Coefficients of
Ellipsoidal and Radial Distances
with Solvent Accessibilities

Protein	residue number	ellipsoidal	radial	g'_2	g'_3	Protein	residue number	ellipsoidal	radial	g'_2	g'_3
1CDZ	96	0.852	0.795	1.56	1.66	1AUN	208	0.672	0.644	1.03	1.39
2RAC	105	0.830	0.788	1.29	1.46	1LBU	213	0.632	0.566	1.70	1.93
1YCC	108	0.821	0.776	1.31	1.50	1YAL	216	0.756	0.685	1.58	1.77
1NEU	115	0.782	0.669	1.93	2.04	2ACT	218	0.744	0.657	1.58	1.75
1DLW	116	0.769	0.700	1.40	1.55	1EUG	219	0.734	0.686	1.28	1.60
1BLO	116	0.752	0.575	2.40	2.60	1AKZ	223	0.736	0.677	1.33	1.59
1DZO	120	0.702	0.517	2.48	2.89	1UDH	228	0.760	0.703	1.39	1.63
1QTS	123	0.815	0.653	2.16	2.21	1TPH	245	0.744	0.712	1.11	1.40
1A4V	123	0.783	0.686	1.87	1.99	1G6V	256	0.754	0.735	1.21	1.31
3LZT	129	0.792	0.682	1.75	1.86	1BN1	257	0.733	0.719	1.22	1.31
1PDO	122	0.831	0.800	1.25	1.45	2DRI	271	0.647	0.455	2.48	2.55
2SNS	141	0.788	0.757	1.34	1.51	1AUA	296	0.620	0.534	1.40	1.48
1ATO	145	0.780	0.737	1.18	1.48	1A3H	300	0.739	0.726	1.17	1.25
1H97	147	0.689	0.608	1.50	1.79	1LDM	309	0.690	0.623	1.63	1.78
1A6M	151	0.728	0.676	1.19	1.61	1FSZ	318	0.715	0.641	1.60	1.69
1I1B	151	0.847	0.825	1.14	1.26	1KFU	338	0.625	0.473	2.23	2.41
1CQ2	153	0.724	0.670	1.13	1.56	1UBY	348	0.578	0.481	1.48	1.89
1PHR	154	0.818	0.795	1.12	1.35	1A26	351	0.655	0.612	1.19	1.52
1CZT	160	0.817	0.762	1.56	1.66	1CTN	356	0.651	0.620	1.11	1.39
121P	166	0.763	0.742	1.13	1.20	1PHC	405	0.573	0.524	1.21	1.61
1B6C	170	0.704	0.666	1.44	1.83	1GAI	448	0.703	0.674	1.28	1.45
1GKY	186	0.670	0.632	1.13	1.43	1BGV	449	0.568	0.535	1.07	1.38
2KFZ	195	0.759	0.722	1.23	1.47	3PBG	468	0.685	0.667	1.14	1.31
1DZV	206	0.765	0.669	2.00	2.03	3COX	500	0.640	0.559	1.63	1.73
1UCH	206	0.805	0.783	1.18	1.36	1FEH	574	0.565	0.487	1.88	2.09

FIG. 3

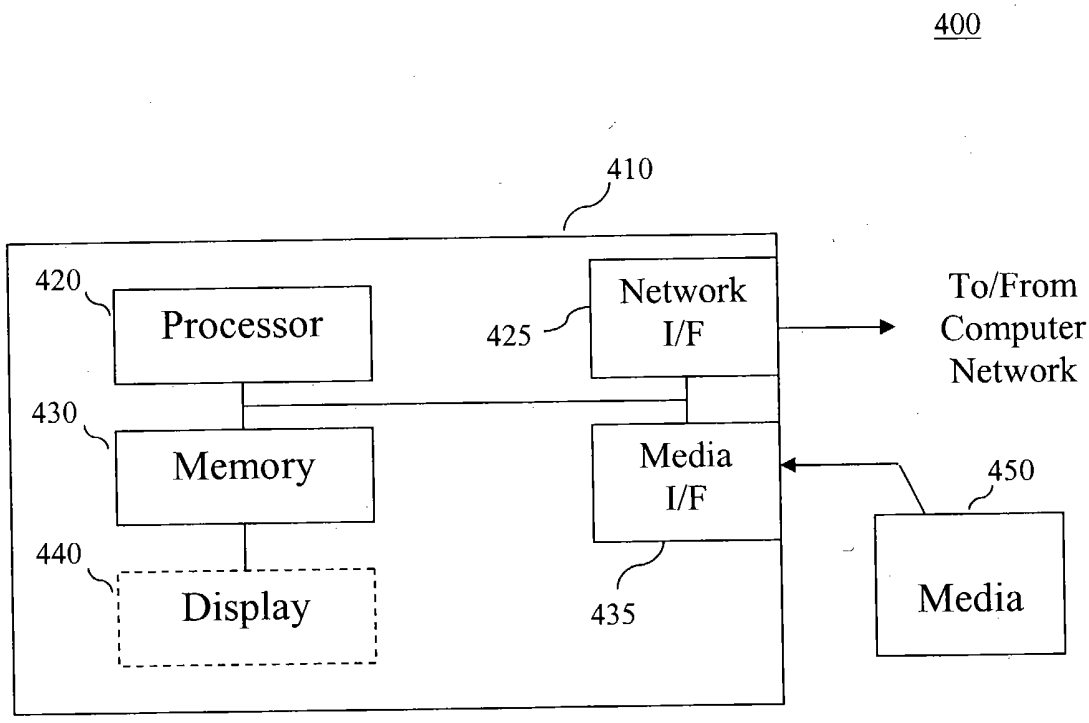
400
410
420
Processor
425
Network
I/F
To/From
Computer
Network
430
Memory
Media
I/F
450
440
Display
435
Media

FIG. 4

Moment Magnitudes and
mean Hydrophobicities

Protein	moment magnitude	random magnitude	number greater	mean hydrophobicity	Protein	moment magnitude	random magnitude	number greater	mean hydrophobicity
1CDZ	6.16	9.49	765	-0.083	1AUN	3.57	6.54	868	-0.122
2RAC	4.24	7.91	864	-0.090	1LBU	3.49	6.82	878	-0.135
1YCC	7.62	8.71	580	-0.222	1YAL	6.58	7.32	565	-0.158
1NEU	8.91	10.24	575	-0.083	2ACT	11.20	7.29	112	-0.092
1DLW	5.97	7.68	677	-0.044	1EUG	5.51	7.41	695	-0.064
1BL0	5.13	10.18	869	-0.164	1AKZ	1.58	7.59	989	-0.105
1DZO	6.29	9.80	762	-0.224	1UDH	6.34	7.39	605	-0.065
1QTS	3.13	10.66	977	-0.063	1TPH	6.92	7.00	491	-0.109
1A4V	9.95	10.64	533	-0.089	1G6V	6.93	7.71	560	-0.154
3LZT	10.35	8.43	269	-0.139	1BN1	6.38	7.62	623	-0.158
1PDO	8.87	8.40	414	-0.047	2DRI	3.26	8.86	943	-0.145
2SNS	6.31	8.15	671	-0.227	1AUA	17.09	7.86	6	-0.134
1AT0	10.11	8.02	242	-0.069	1A3H	1.83	6.57	975	-0.131
1H97	5.22	8.94	631	-0.110	1LDM	13.81	7.90	65	-0.039
1A6M	3.41	8.73	943	-0.117	1FSZ	4.83	7.48	784	-0.089
1I1B	3.92	8.76	915	-0.150	1KFU	11.05	8.88	281	-0.118
1CQ2	3.79	8.47	922	-0.122	1UBY	8.84	8.27	412	-0.104
1PHR	5.20	8.04	770	-0.121	1A26	5.44	7.44	725	-0.117
1CZT	9.91	9.16	395	-0.120	1CTN	2.78	6.73	937	-0.124
121P	7.68	7.80	478	-0.134	1PHC	3.67	7.23	880	-0.087
1E6C	9.54	8.71	366	-0.054	1GAI	5.79	6.07	522	-0.114
1GKY	9.63	8.43	332	-0.170	1BGV	7.75	6.40	296	-0.100
2KFZ	6.82	8.07	594	-0.096	3PBG	5.82	6.34	544	-0.121
1DZV	15.31	8.41	40	-0.042	3COX	4.32	6.95	806	-0.120
1UCH	10.39	7.90	232	-0.094	1FEH	6.92	7.60	567	-0.129

FIG. 5

Neumaier Hydrophobicity scale

amino acid	hydrophobicity	amino acid	hydrophobicity
LYS	-1.00	HIS	-0.15
ASP	-0.97	ALA	-0.06
GLU	-0.85	TYR	0.35
ARG	-0.80	CYS	0.56
GLN	-0.71	TRP	0.57
ASN	-0.70	MET	0.68
SER	-0.48	VAL	0.75
PRO	-0.45	LEU	0.83
THR	-0.38	PHE	0.99
GLY	-0.32	ILE	1.00

FIG. 6

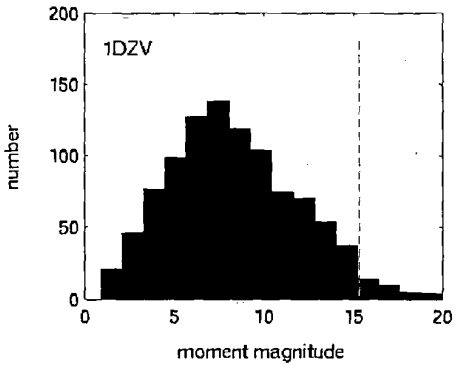
1DZV
number
moment magnitude
0
50
100
150
200
0
5
10
15
20

FIG. 7A

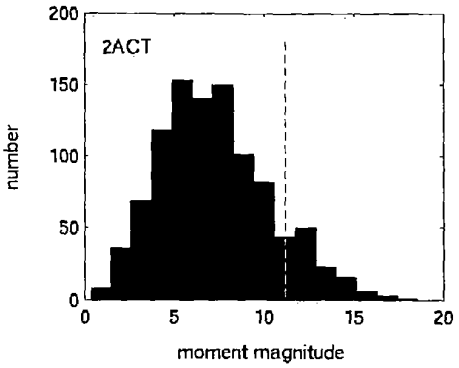
2ACT
number
moment magnitude
0
50
100
150
200
0
5
10
15
20

FIG. 7B

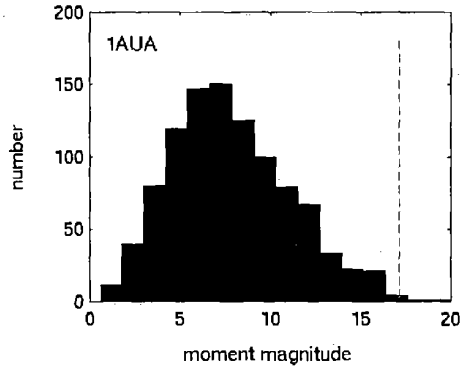
1AUA
number
moment magnitude
0
50
100
150
200
0
5
10
15
20

FIG. 7C

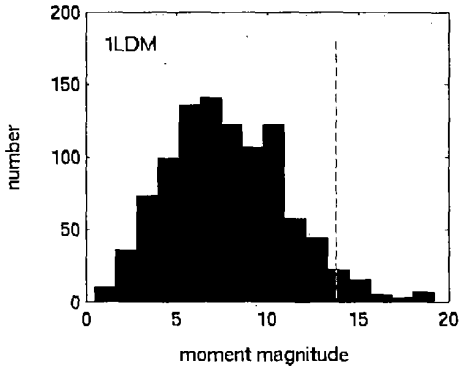
1LDM
number
moment magnitude
0
50
100
150
200
0
5
10
15
20

FIG. 7D

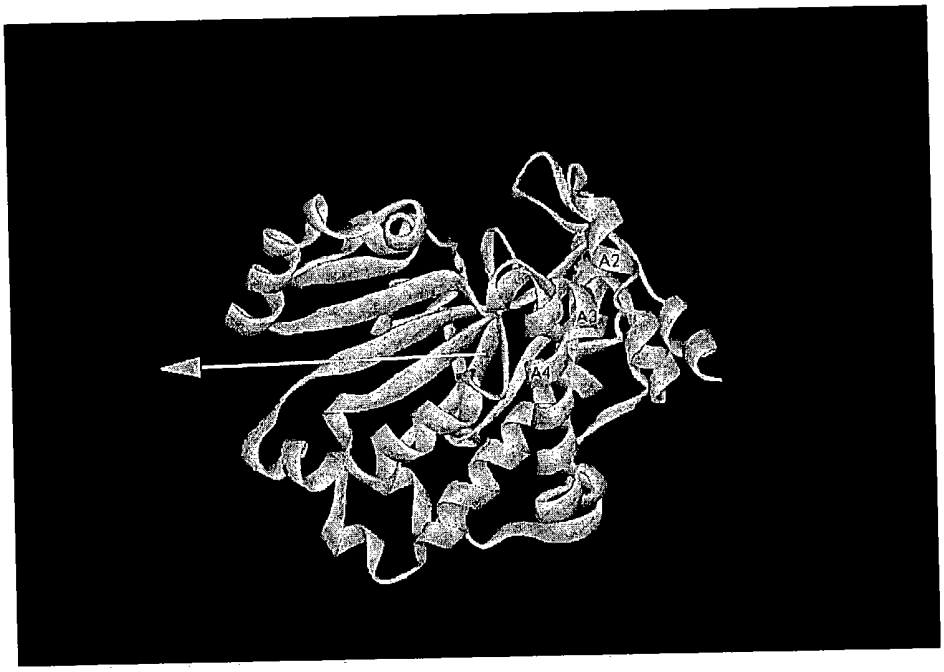

FIG. 8

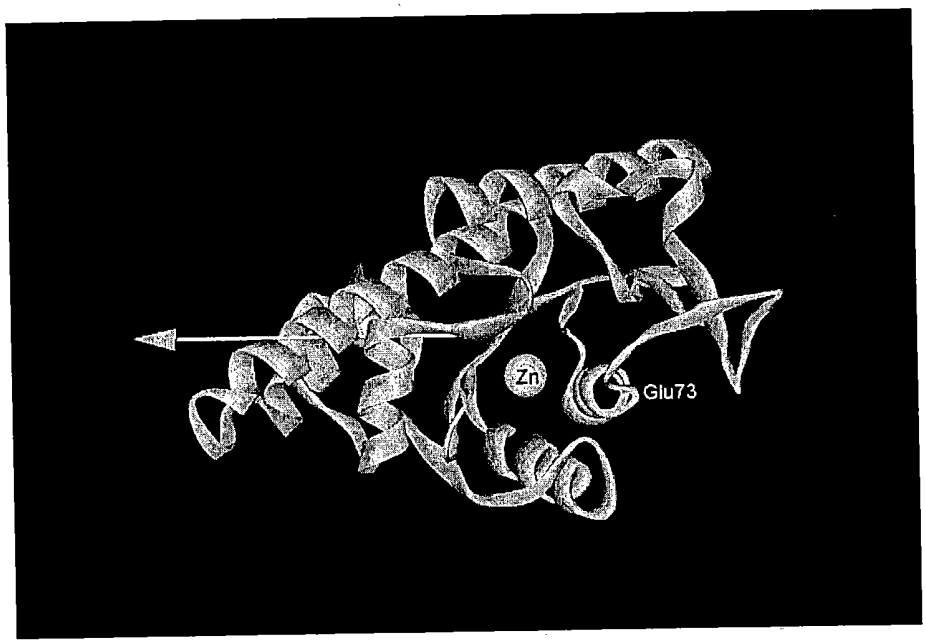

FIG. 9

Defensin and Defensin like
Moment Magnitudes and
mean hydrophobicities

Protein	moment magnitude	random magnitude	number greater	mean hydophobicity	g'_2	g'_3
1AHL	16.86	9.09	24	-0.089	1.85	2.02
1APF	23.16	10.55	31	-0.100	1.20	2.66
1B8W	15.79	18.98	539	-0.182	1.97	5.34
1BNB	13.58	17.00	615	-0.001	3.13	4.96
1DFN	3.34	9.25	955	0.070	2.29	2.44
1FD3	5.74	9.35	806	-0.079	1.97	2.36
1FJN	7.02	12.37	745	-0.076	1.64	3.96
1SH1	36.35	13.60	9	-0.184	1.98	3.60

FIG. 10

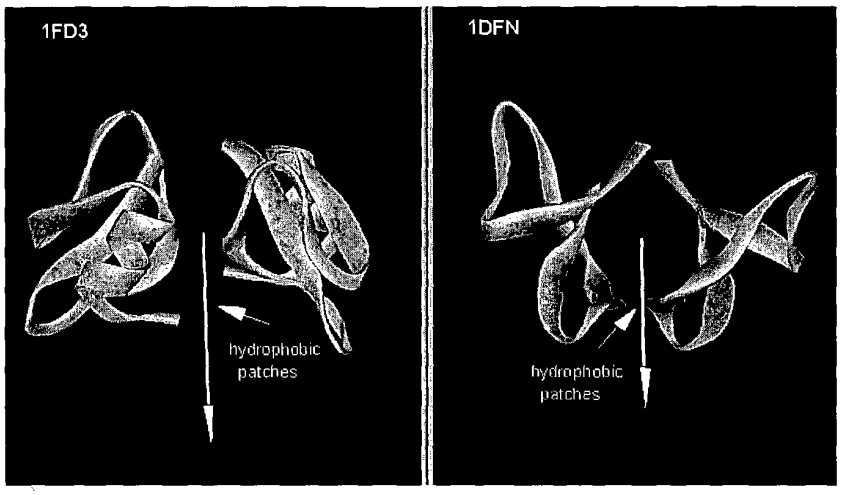

FIG. 11A

FIG. 11B